Conduction band valley splitting in silicon nano-structures

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A theory based on localized-orbital approaches is developed to describe the valley splitting observed in silicon nano-structures. The theory is appropriate in the limit of low electron density and relevant for proposed quantum computing architectures. The valley splitting is computed for realistic devices using the quantitative nanoelectronic modeling tool NEMO using the empirical tight binding model $sp^3d^5s^*$. The empirical tight binding parameters have been fitted to bulk bandstructure behavior of Si using a genetic algorithm. Focal points of the empirical fit are the effective masses and bandedges in the lowest conduction band and the upper valence bands with particular attention to effects of hydrostatic and bi-axial distortions.

A simple 1-D quantum well simulation in NEMO shows the basic features of conduction band valley splitting as a coherent, confinement-induced phenomenon. No additional intervalley scattering parameters are needed. To explore the physics in more detail a simple, analytically solvable tight-binding model, which reproduces the behavior of the splitting in the NEMO results, is developed. The splitting is in general nonzero even in the absence of electric field in contrast to previous works. The splitting in a square well oscillates as a function of N, the number of layers in the quantum well, with a period that is determined by the location of the valley minimum in the Brillouin zone. The envelope of the splitting decays as N^3. The qualitative physics remain the same irrespective of the details of the quantum well boundaries or the details of the strain treatment in the quantum well.

The realistic modeling of qubits in a strained Si quantum well grown on top of relaxed SiGe modulated by 2-D surface gates requires the simulation of the electrostatic potential profile in the extended heterostructure in 3-D. The device region is too large to be treated in the purely atomistic NEMO 3-D approach. First results of a hybrid approach in which the potential is computed on a mesoscopic scale in an envelope function approach and the electronic structure is computed in an atomistic approach are presented. Preliminary results show a valley splitting of s-like ground states of the order of 0.5meV. Evaluation of magnetic field effects show a further state splitting which is about one order of magnitude less. Higher lying orbital states such as p_x and p_y are higher in energy by a splitting of the order of a few meV. The valley splitting is therefore shown to be large enough to provide a large enough state separation to enable quantum computing in the lowest valley split state that is split by magnetic fields.

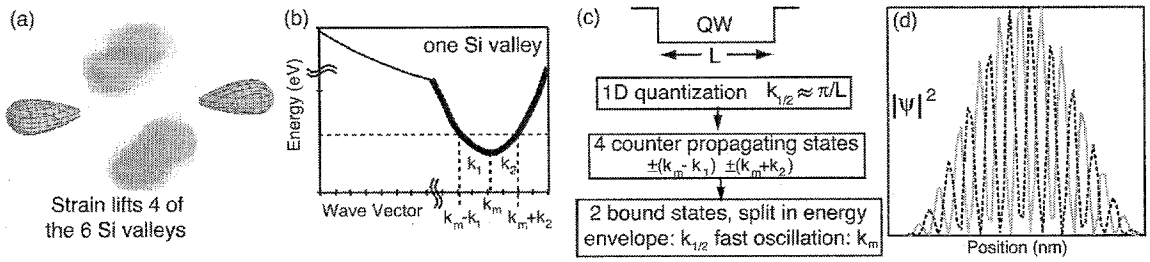

Figure 1: (a) Sketch of Electron dispersion isosurface of Si. 4 valleys are raised due to bi-axial strain. (b) Zoom of dispersion on one valley. One constant energy corresponds to two wavevectors. (c) sketch of 1-D quantization creating 2 bound states. (d) 1-D wavefunctions indicating an s-like envelope and 2 orthogonal fast oscillations.

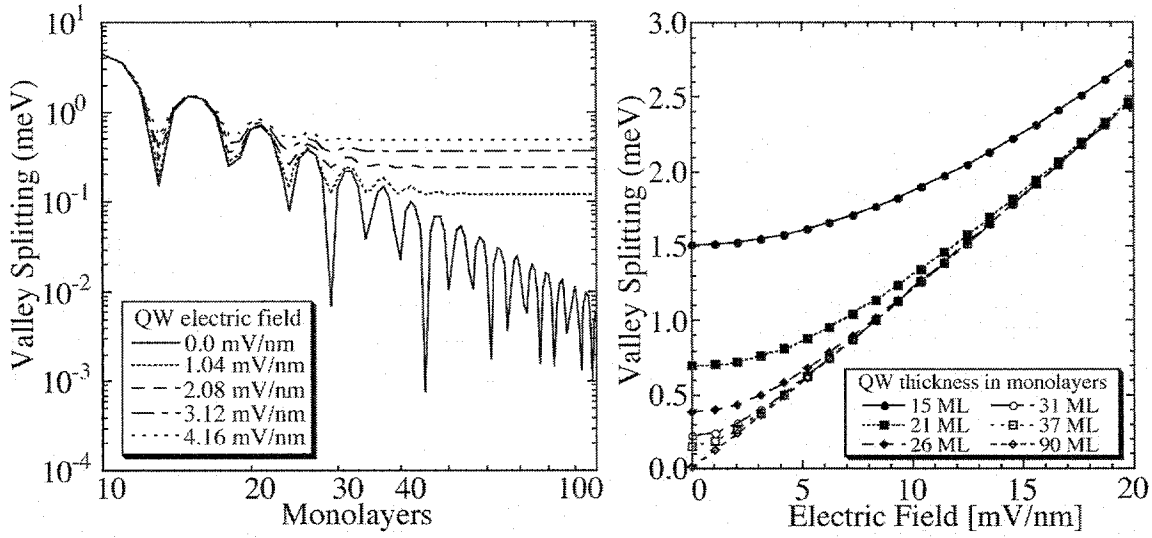

Figure 2: (a) Valley splitting versus well width at various applied fields for a strained Si quantum well with hardwall boundary conditions, calculated using NEMO's nearest-neighbor spin-orbit $sp^3d^5s^*$ model. Although calculations are only for integral numbers of monolayers, lines are used as a guide to the eye. (b) Valley splitting in a strained Si quantum well with hardwall boundary conditions versus applied field for several well widths in monolayers. The particular monolayers correspond to peaks in the solid curve of (a). Actual points calculated are shown as symbols.

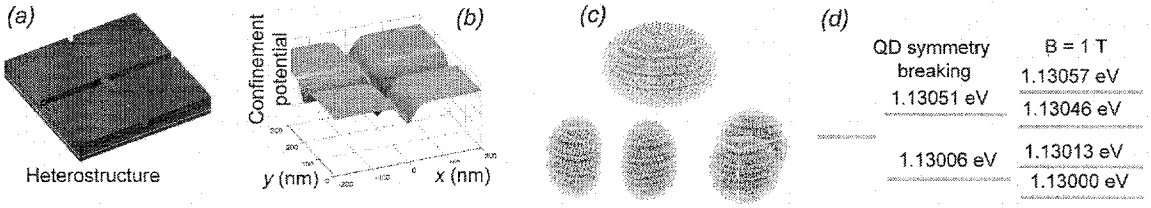

Figure 3: Hybrid approach to modeling of qubits in SiGe system. (a) 3-D heterostructure. (b) Mesoscopic potential profile. (c) Atomistic wavefunctions. (d) Energy spectrum due to valley splitting and magnetic field. Orbital splitting shown in (c) is significantly larger in energy than the lowest levels shown in (d).

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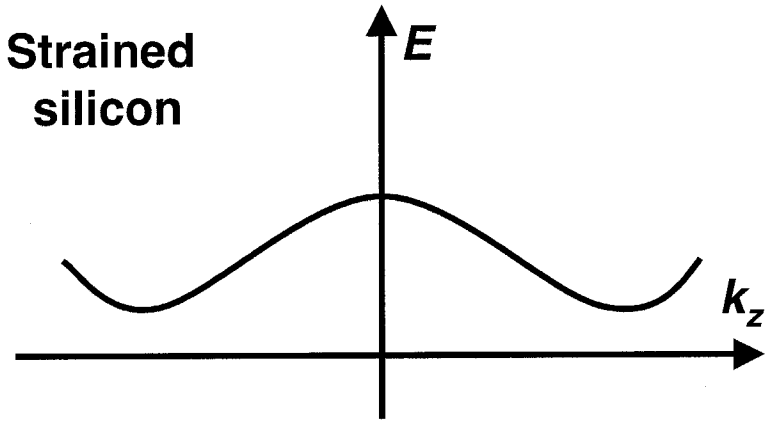
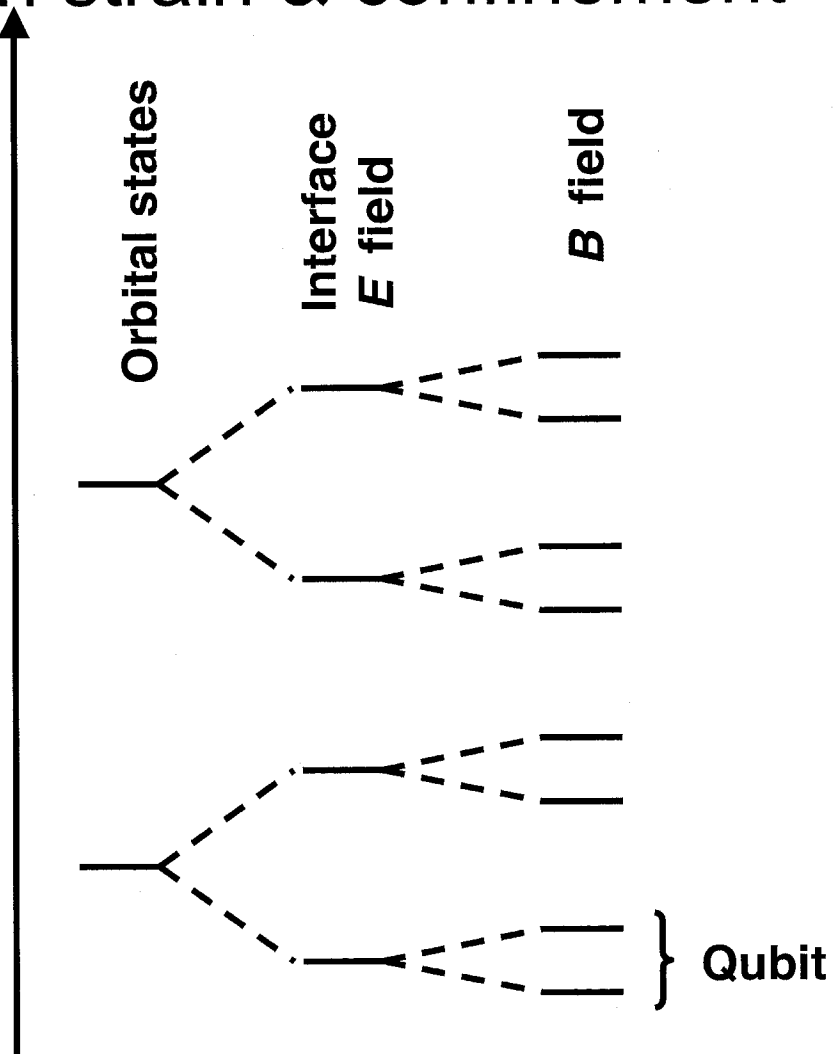
Quantum Dot Quantum Computing in Si:
Lifting Degeneracies with strain & confinement



Valley degeneracy in X direction is broken by interface and electric field

Are the qubit states separated enough from higher energy states?



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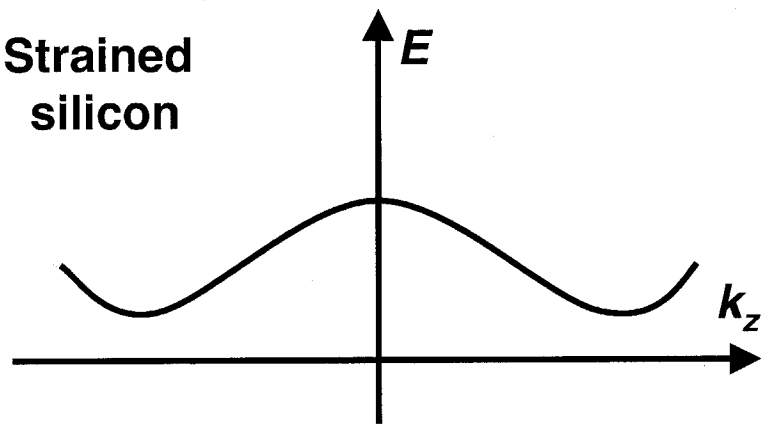
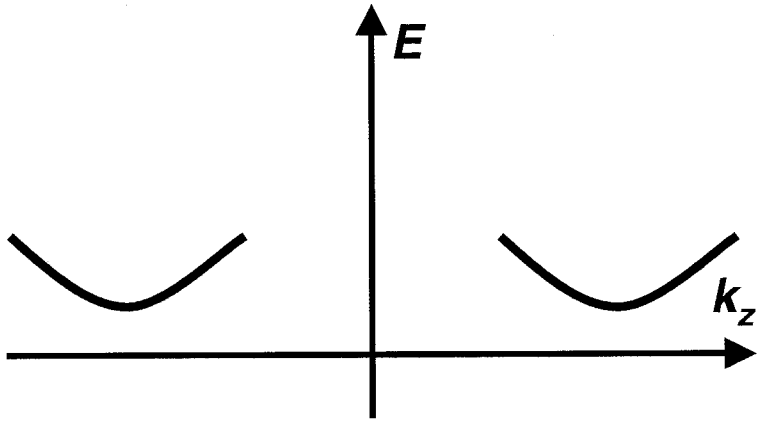




Valley degeneracy in X direction is broken by interface and electric field

Atomistic deliver these details automatically.

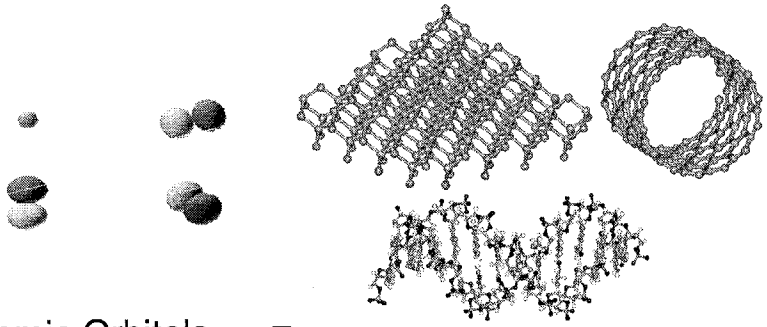
Standard Approach:

Effective Mass

Single, parabolic band

Need high-powered physics, (hand-waiving) coupling constant to couple the valleys.

Mapping of Orbitals to Bulk Bandstructure



Atomic Orbitals
size: 0.2nm

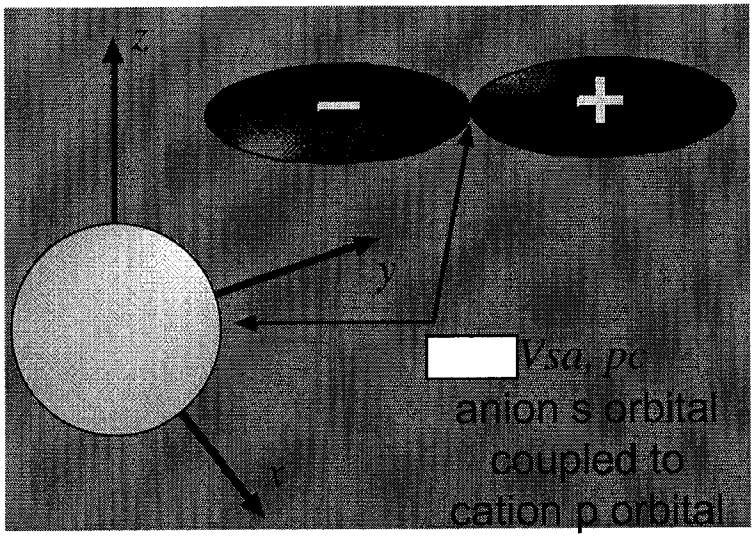
Structure

Bulk Semiconductors are described by:

- Conduction and valence bands, bandgaps (direct, indirect), effective masses
- 10-30 physically measurable quantities

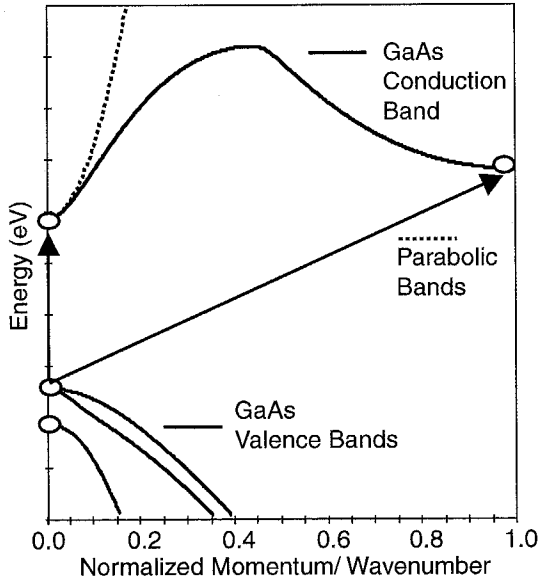
Tight Binding Models are described by:

- Orbital interaction energies.
- 15-30 theoretical parameters



High Dimensional Fitting Problem

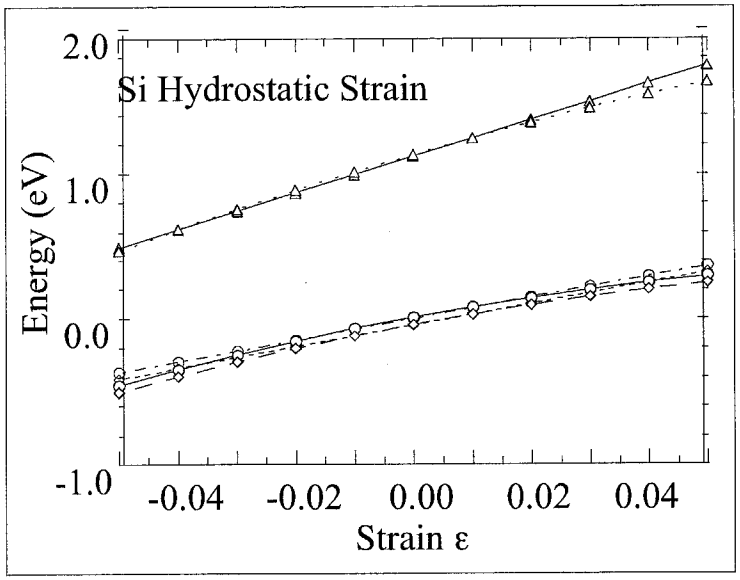
Numerical and analytical approach developed

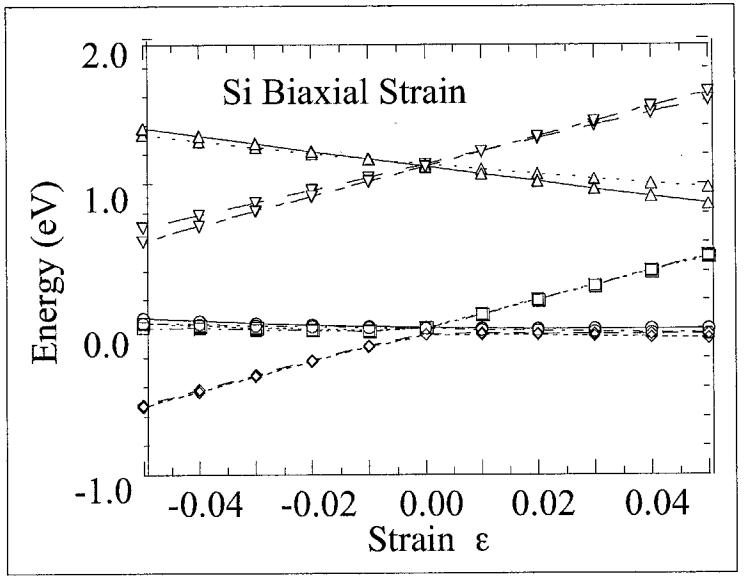


15-30 theoretical interaction energies

10-30 data points of bands and masses

Bulk Si: Strain Behavior

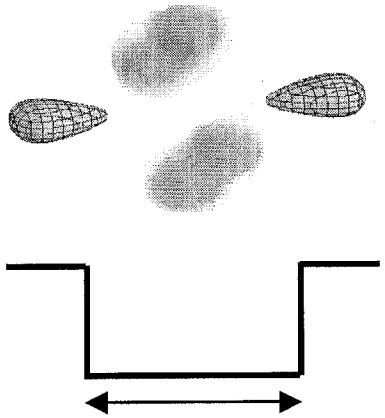




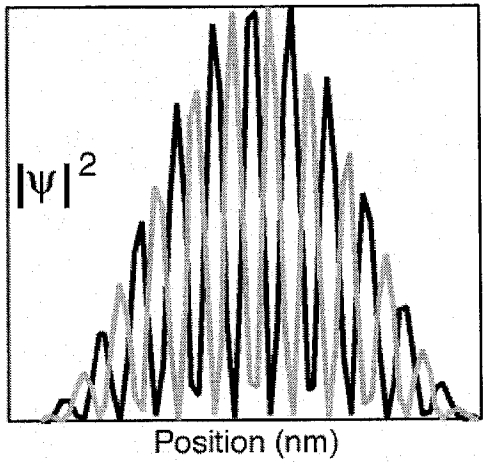
Hydrostatic distortions:
match k.p theory and experiment

Bi-Axial distortions:
match k.p theory and experiment

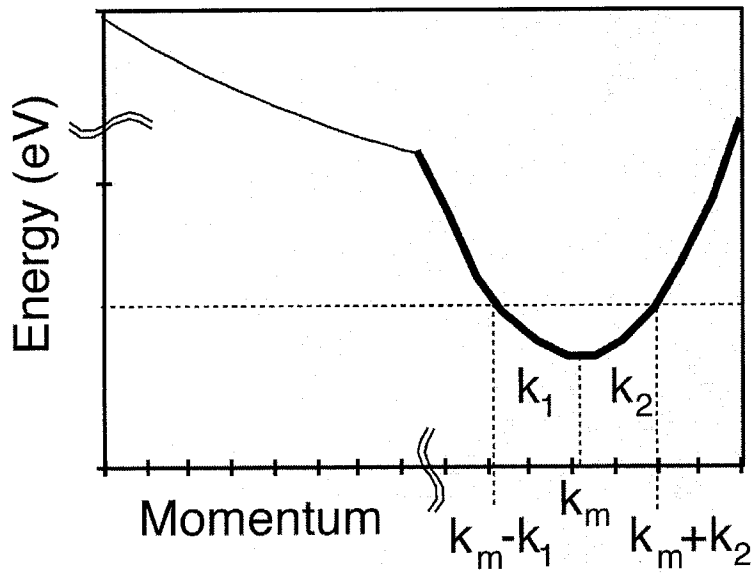
1D Confinement Creates Valley Splitting:



$k=\pi/L$



Valley Splitting ΔE~1meV



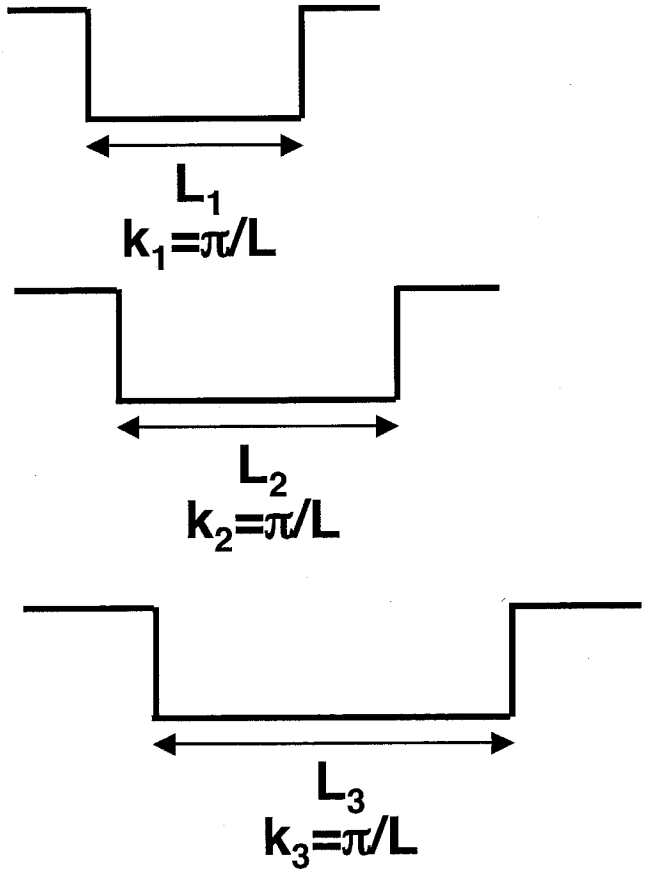
4 propagating states

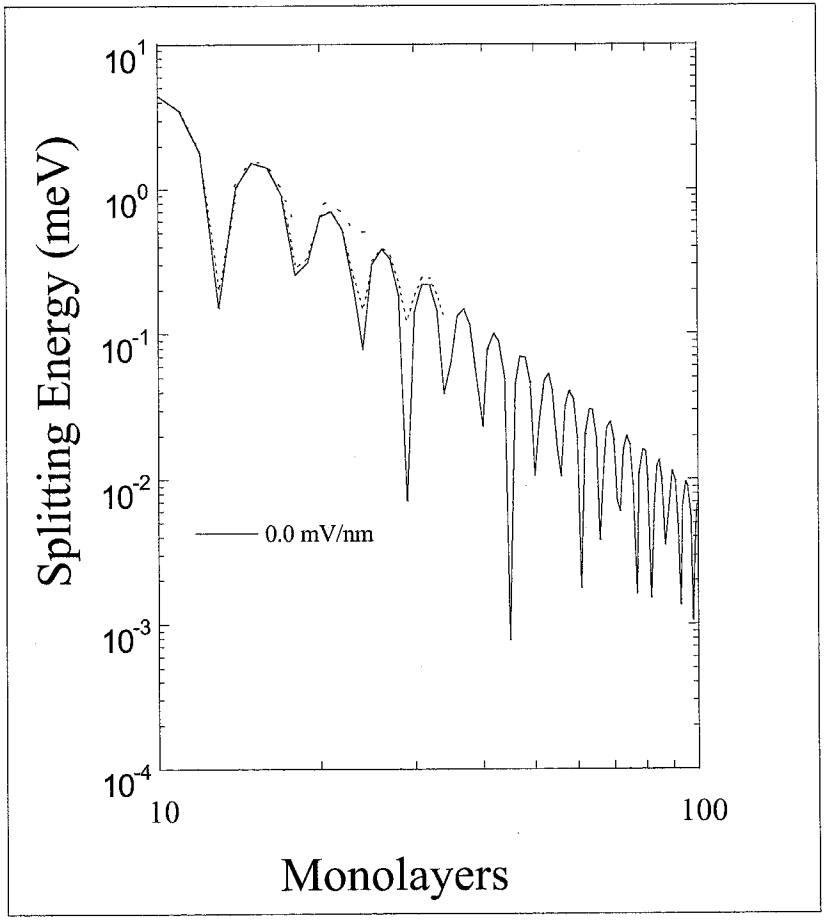
↓

2 bound states
$k_{1,2}$ envelope
k_m fast oscillations

Splitting Behavior With Quantum Well Width

- Strained Si QW, Hardwall BCs
- Oscillations with Monolayers (decay as ML^{-3})





Splitting Behavior With Quantum Well Width and Electric Field

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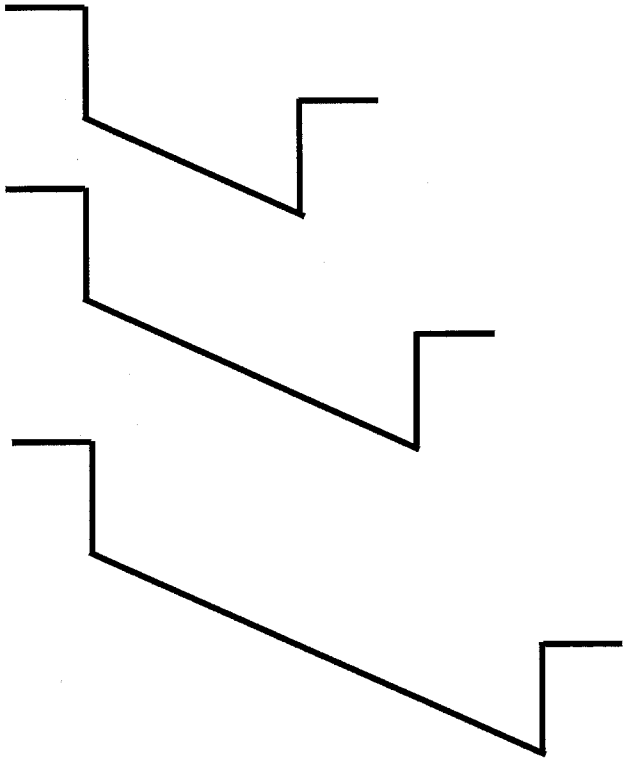
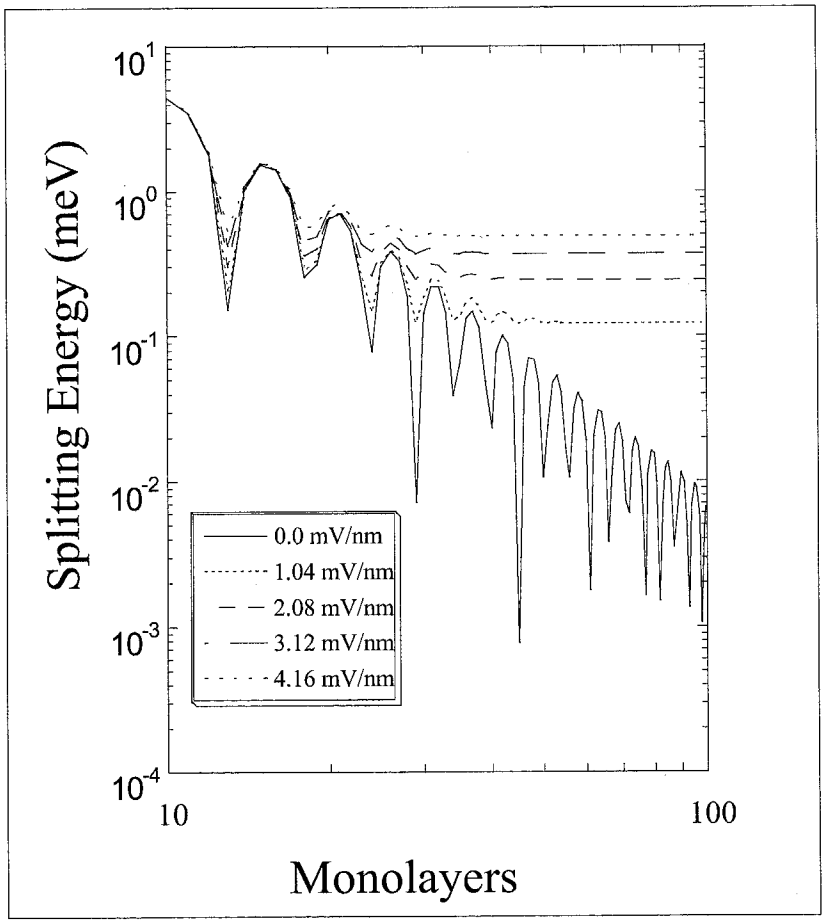
- Oscillations with Monolayers
- Oscillations decay with increasing Field
- Decay significant once drop/ML is of order zero-field splitting





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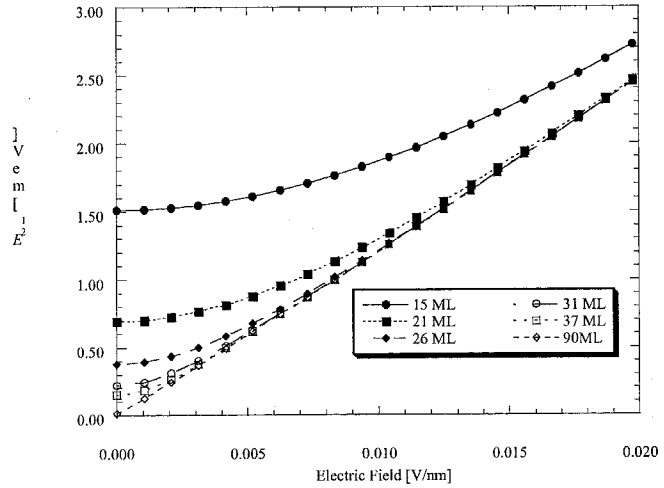

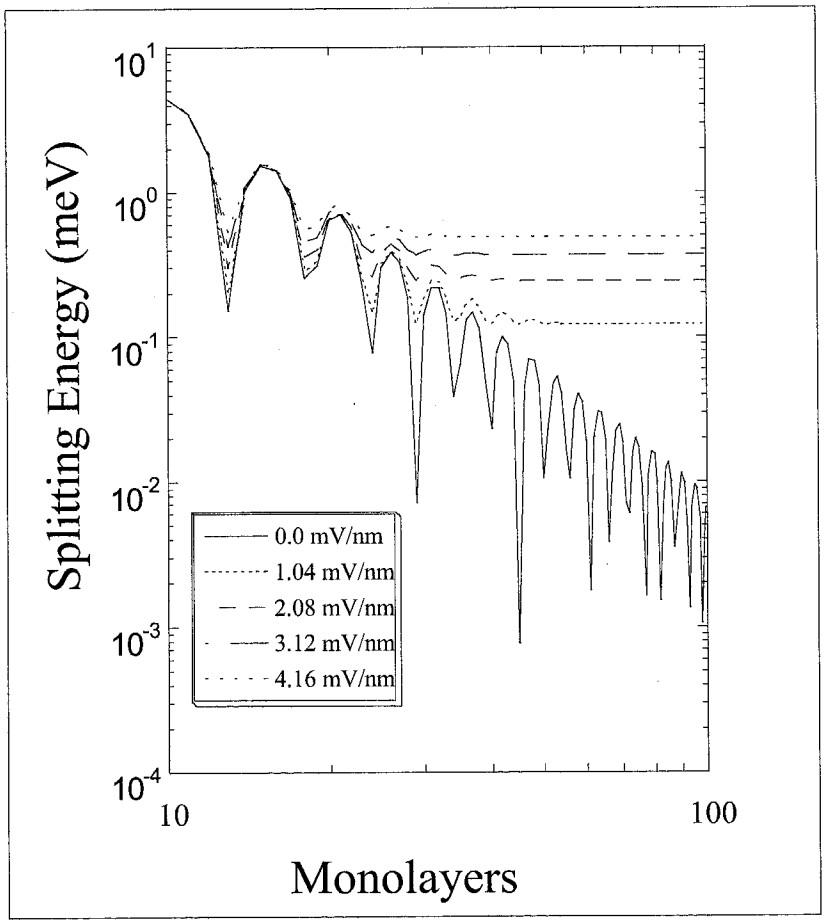

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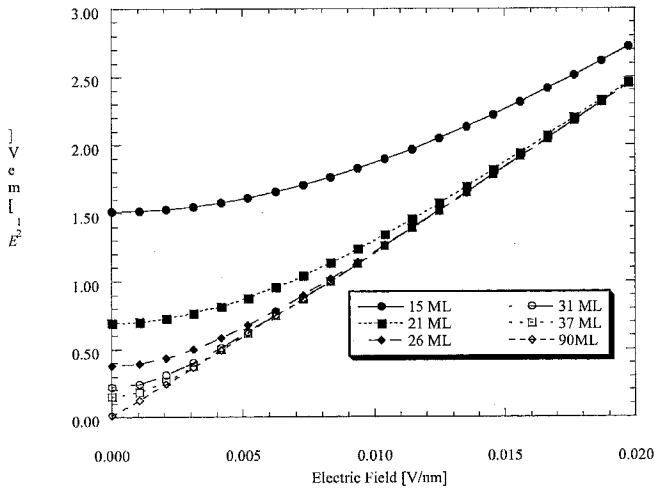
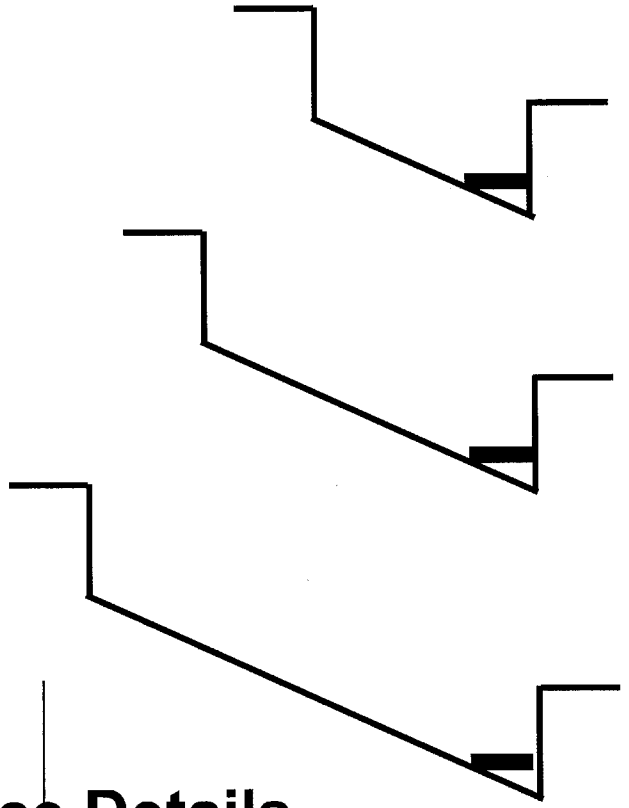




Device Details (structure, materials, local fields,) determine energy splitting

Hybrid Approach to Valley Splitting in 3D Qubits

Problem:

- Valley splitting is strongly affected by local, inhomogeneous *E* fields that are not necessarily parallel to ***z***.

⇒ Requires 3D treatment.

- Atomistic approach, including gates and heterostructure, is too large for NEMO3D alone.

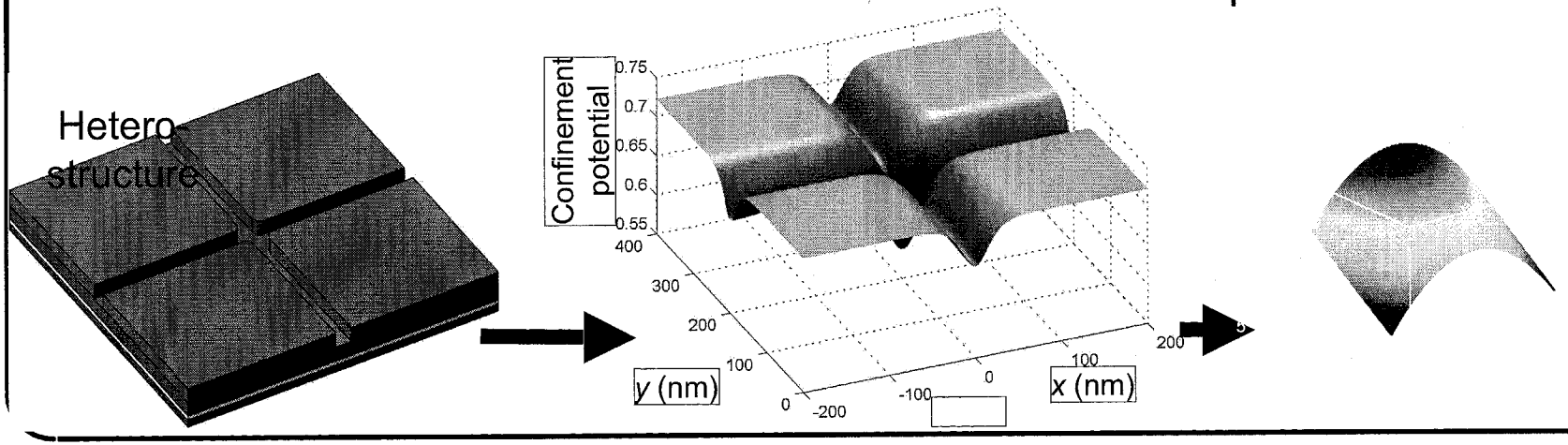
⇒ Hybrid mesoscopic/atomistic simulations.

Approach:

- Electrostatic potentials, including gate and image potentials, self-consistency, are computed at Wisconsin for hetero-structures with envelope functions.

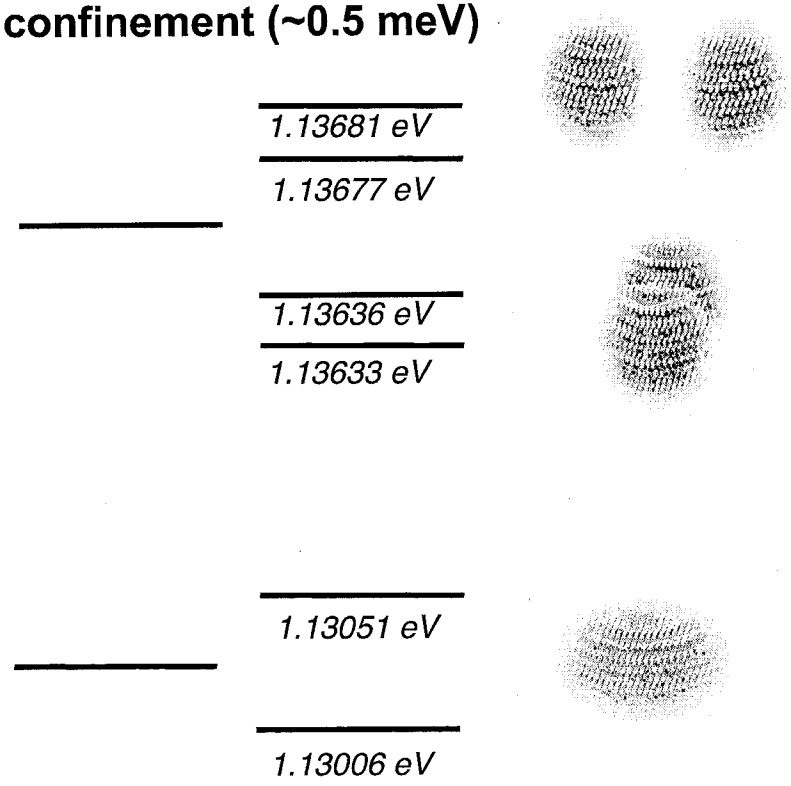
Potentials, Envelope functions	Wisconsin
⇓	
Wavefunctions, Valley splitting	JPL

- NEMO3D computes exact wavefunctions in quantum dot.

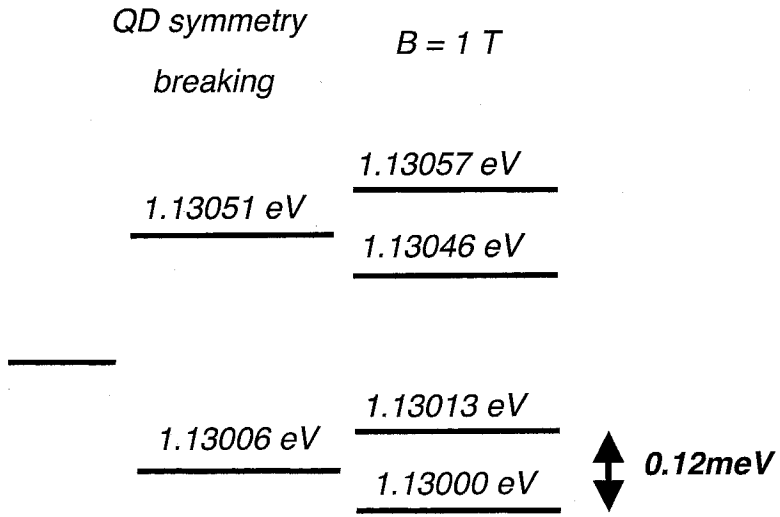


Relative Size of State Splitting
3-D Electronic structure of low-lying states

- Valley splitting due to breaking of translational invariance is typically smaller than splitting due to confinement (~0.5 meV)



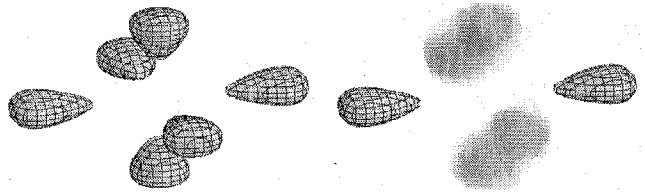
- Even with a large B=1.0T, Zeeman splitting is much smaller than valley splitting (~0.12 meV).



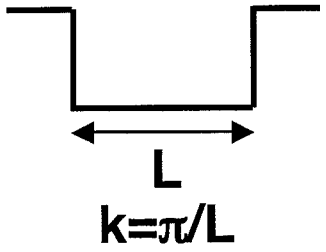
Quantum Dot Quantum Computing in Si:

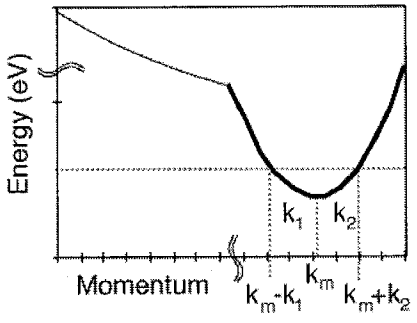
Lifting Degeneracies - strain & confinement

- **Bi-axial strain on Si.** **Lifting 4 of the 6 degenerate valleys ΔE>100meV**



- **Confinement in 1D:** **Valley Splitting ΔE~1meV**





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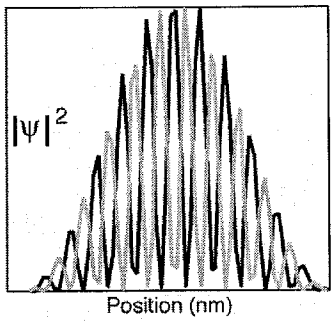

- **Confinement in 3D:** **(1D heterostr. & 2D lat gates & mag. field) ΔE~0.1meV**